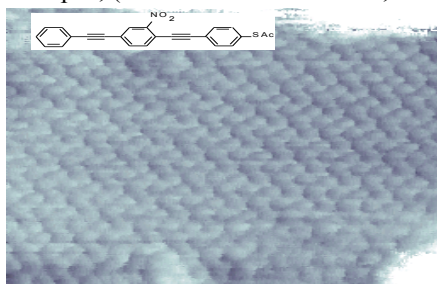


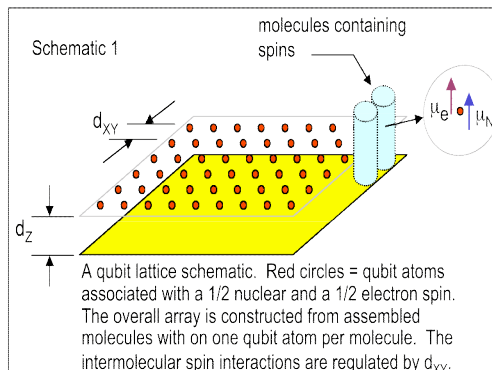
## Self-Assembled Quantum Computers and Hybrid Quantum Computers

**SAM:** G.P. Berman (T-13), G.D. Doolen (T-13), V.I. Tsifrinovich (NY Polytech. U.), D.L. Allara (Penn. S.U.), J. Tour (Rice U.), S. Tretiak (LANL, T-6), A. Tamulis (Lithuania and T-13/CNLS).

**Type-II QC:** G.P. Berman (T-13), G.D. Doolen (T-13), A.A. Ezhov (Fusion Research In., Russia), D.I. Kamenev (T-13/CNLS), J. Yepez, (Air Force Research Lab., Hanscom Field, MS).



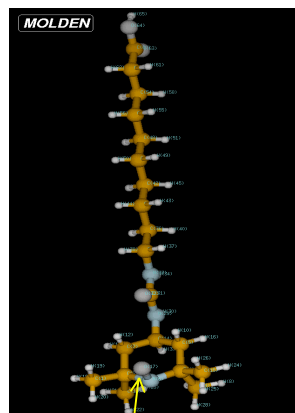
10x10 nm STM image of a monolayer of a TR molecule (Weiss, Dornhauser, Stapleton, Allara, unpublished results).



## Scalable spin-based quantum computer: First principles calculations and modeling of decoherence time in SAMs

- Quantum calculations of molecular vibrational normal modes (phonon spectrum) with Density Functional Theory (DFT) and/or correlated approaches (e.g. HF/MP2)
- Calculation, analysis, and comparison with experiment of Raman and IR spectra
- We will calculate spin-orbit interaction to model spin decoherence induced vibrational dephasing. (This will allow us to formulate an effective Hamiltonian model to simulate time-dependent dynamics and relaxation of a single qubit.)
- We will calculate dipolar coupling between spins in self-assembled aggregates using typical SAM morphologies as an input to quantum-chemical calculations.
- Decoherence time is expected to be increased in finite molecular systems because of the discrete nature of phonon spectrum.**

Attached to the substrate



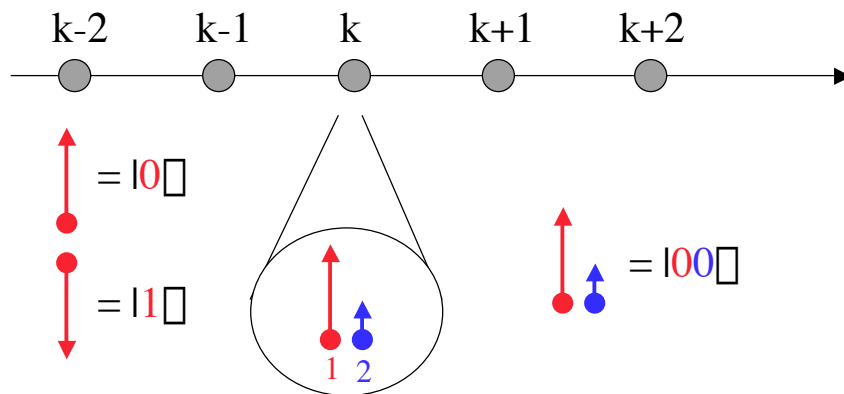
Oxygen, spin 1/2

**Stable spin electron  
nitroxyl radical**

## Quantum Institute Workshop

Quantum Institute Briefing Center; December 9–10, 2002

Type-II quantum computer — Quantum lattice gas algorithm for simulation of diffusion equation.



$$\rho(x_k, t) = \rho_1(x_k, t) + \rho_2(x_k, t) - \text{mass density}$$

$\rho_1(x, t)$  is the probability to find the red spin in the state  $|1\rangle$

$\rho_2(x, t)$  is the probability to find the blue spin in the state  $|1\rangle$

**Presenter: Gary Doolen**